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16. ABSTRACT

This paper documents two dense gas projects undertaken at the US EPA Fluid Modeling Facility. The study investigated the basic nature of the transport and dispersion of a dense gas plume in a simulated neutral atmospheric boundary layer. The two dense gas releases were CO_2 which is 1.5 times as dense as air and SF_6 which is 5.2 times as dense as air. The configuration of the wind tunnel was the same for both gases except that the wind speed had to be increased 20% in the SF_6 study to avoid laminarization of the plume. The plumes were tracked by mixing a samll fraction of ethane with the dense gases and using flame ionization detectors to measure downwind lateral and vertical concentration profiles. The increaed density clearly has very significant effects. The vertical spread of the SF_6 plume was about two-thirds that of the CO_2 plume, and the lateral spread was initially twice that of the CO_2 plume. Perhaps the most unusual finding was that the shapes of the vertical distributions remained similar far downstream and highly non-Gaussian in the outer reaches of the plume.

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INTRODUCTION

In view of numerous accidental releases of toxic gases into the atmosphere in recent years, there is increasing concern regarding the atmospheric dispersion of toxic and hazardous materials. Given that exposures to the toxic substances could be life threatening or severely incapacitating, there is an urgent need to develop and validate modeling approaches relevant to the atmospheric dispersion of airborne toxic material. Tools for modeling re-leases of toxic materials into the atmosphere that involve neutrally buoyant non-reactive chemicals are already available. However, many hazardous chemicals are heavier than air and tend to hug the ground and not mix well with the ambient air. These releases may be due to evaporation of highly volatile liquids or venting of pressurized vessels, which may be significantly affected by the buoyancy forces. The available experimental data suggest that these types of releases displace the atmospheric flow in the near-field, resulting in increased dwell time of the cloud at any particular location.

Dispersion processes of heavier-than-air gases in the atmosphere are significantly different from those of trace contaminants. The presence of a trace contaminant is assumed not to affect the atmospheric flow fields and, therefore, the distribution of trace contaminants is the result of transport and turbulent dispersion in the atmospheric boundary layer. In contrast, the release of a large quantity of a dense gases into the atmosphere may alter the atmospheric flow in the immediate vicinity of the release resulting in reduced transport and cloud dispersion by the ambient turbulent motion. For such releases the gravity-induced flow and the resulting interaction with the atmospheric flow determine the shape and extent of the area which is subject to flammable or high doses of toxic gas.

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The object of this paper is to illustrate the transport and dispersion resulting interaction with the atmospheric flow determine the shape and extent of the area which is subject to flammable or high doses of toxic gas. characteristics of dense-gas plumes using data collected in a wind tunnel, and to test the performance of two available dispersion models with the CO_2 and SF_6 concentration data from the wind-tunnel experiments. Specifically, DEGADIS and INPUFF 2.2 are evaluated against this experimental data base. It is not the intent of this paper to provide an exhaustive evaluation of atmospheric dispersion models appropriate to heavier-than-air releases. Rather we choose to compare one state-of-the-art dense-gas model with a Gaussian puff model which is appropriate for neutrally buoyant releases. Although the simple Gaussian models do not incorporate the relevant physics for dense gas spread and diffusion, they may be useful in estimating ground level center-line concentrations from a surface release.

The two dense gas experiments were undertaken at the U.S. EPA Fluid Modeling Facility. The general experimental setup and data collection procedures are provided in Britter and Snyder, 1986; Britter and Snyder, 1988; and Snyder, 1987. CO_2 with a specific gravity of 1.52 was used as the effluent in the first experiment. In the second, the effluent was SF_6 (sulfur hexafluoride), which has a specific gravity of 5.11. Sulfur hexafluoride was chosen as the result of a survey of possible source gases and because of its large density, low toxicity (no known harmful effects at any concentration levels) and low cost. Although other gases met the density criterion, they were either toxic, harmful to the ozone layer in the atmosphere (such as freons), or exorbitantly expensive (such as xenon). SF_6 is 3.36 times as dense as the CO_2.

EXPERIMENT

The basic configuration of the wind tunnel was the same for both CO_2 and SF_6. A honeycomb was in position at the entrance to the test section (3.7 m wide, 2.1 m high, and 18 m long). A 153 mm high fence stretched across the tunnel floor at a location 650 mm downstream of the exit plane of the honeycomb in order to generate a simulated atmospheric boundary layer 1 m deep. The floor downwind of the fence was covered with 10 mm gravel (Sanspray). The source was positioned 7986 mm downwind of the fence, beyond which the boundary layer was in approximate equilibrium. Sufficient measurements of the boundary layer structure and its dispersion characteristics were made to ensure its similarity to the neutral atmospheric boundary layer.

The source geometry for both experiments was a circular area source with a 104 mm diameter. This configuration was chosen such that the surface roughness was maintained homogeneous across the entire floor of the tunnel, including the source itself. The efflux velocity was thus essentially uniform over the area source, with a value of approximately 6.1 cm/s, a little larger than the friction velocity at the nominal free-stream velocity of 1 m/s.

The plume was tracked by mixing a small fraction of ethane (C_2H_6) with the dense gas and using flame ionization detectors (FID's) to measure concentrations downstream. The ethane flow rate was maintained at 900 cc/min (or 300 cc/min) and the dense gas at 30,000 cc/min. These rates were measured using laminar flow elements (LFE's) and micromanometers. The LFE's were calibrated in situ using the respective gases, regulators, values, tubing, etc., and a Brooks flow calibrator (floating pistons in glass tubes with mercury seals).

Under low enough wind speeds and strong enough stable density gradients (created by the surface releases of dense gases), the plumes had tendencies to laminarize, which is not a realistic simulation of a full-scale dense gas release. To ensure that laminarization did not occur, flow visualization was done prior to the quantitative measurements. The plumes were visually observed (through injection of smoke) over a range of wind speeds to ascertain whether their basic character was laminar or turbulent. The lowest wind speeds at which the plume appeared fully turbulent were approximately 0.95 m/s for the CO_2 plume and 1.1 m/s for the SF_6 plume (laminar streaks were observed at lower wind speeds). Hence, these wind speeds were used during the quantitative measurements. These wind speeds were the smallest that could be used (hence, providing the most significant buoyancy effect) while maintaining fully turbulent plumes.

PRESENTATION AND DISCUSSION OF RESULTS

Figure 1 shows the measurements made of center-line longitudinal concentration profiles with SF_6 as the source gas. The first profile was measured using a spring-loaded rake with the plates on the bottom, so that the effective sampling height was 5 mm above the tops of the rocks. Because of the apparent large scatter close to the source, this profile was repeated. Note that the apparent scatter is still quite large, but highly repeatable. The rake was then replaced by a bent tube that was brought to the surface (touching the rocks) for each measurement. This profile displayed considerably larger concentrations (by factors as large as 2.5) close to the source and much less scatter. These strong differences are attributed to the extremely strong gradients of concentration in the vertical direction; as will be shown below, an elevation difference of 5 mm in the sampling height could easily account for a change by a factor of 3 in the measured concentration. Finally, in order to make measurements all the way across the source itself as well as upstream, the source concentration was reduced to 1% ethane (in SF_6). This profile may be seen to match the previous profile when scaled by a factor of 3. Because the zero and negative values cannot be shown the logarithmic plot of Figure 1, the last two profiles are replotted on Figure 2 using semilogarithmic axes. The match between the two profiles is regarded as excellent.

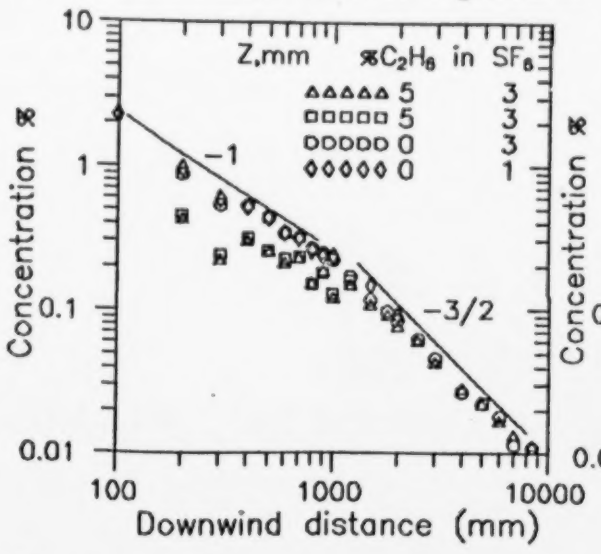

Fig. 1. Longitudinal concentration profile measurements with SF_6 as source gas.

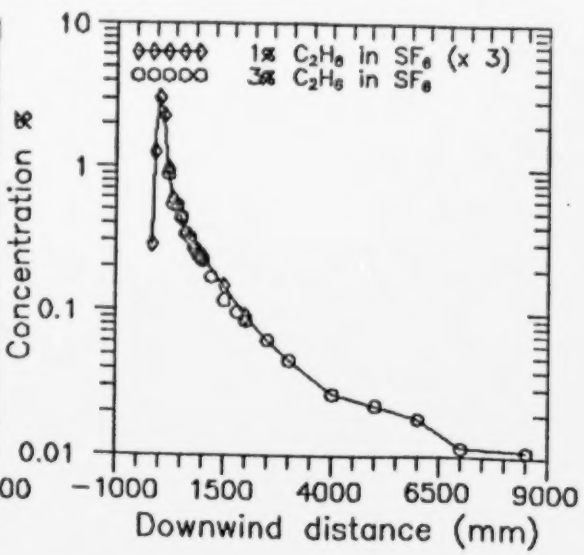

Fig. 2. Longitudinal concentration measurements through the source with SF_6 as source gas.

Comparison of the longitudinal concentration profiles of CO_2, SF_6, and air is shown in Figure 3. We have scaled the concentrations by the source concentration, and, have multiplied the indicated CO_2 concentrations by 0.9 because of the synergistic effect of the CO_2 on the FID response. The profiles are quite similar in shape. The larger differences in CO_2 and SF_6 close to the source are most likely attributable to the somewhat different sampling elevations, the CO_2 having been measured at an effective elevation of 5 mm and the SF_6 at "ground level". If these concentrations had been scaled in the way normally applied by air pollution meteorologists (i.e., $\chi U/Q$), the two profiles would be spread apart even farther (by the ratio of the wind speeds, about 18%).

A direct comparison of the vertical concentration profiles of SF_6, CO_2 and air (at x = 600 mm) is shown in Figure 4. Note that, in spite of the different wind speeds and very different densities and vertical distributions, the surface concentrations are essentially identical. The larger density of the SF_6 is clearly significant, however, as the shapes of the vertical distributions are qualitatively different for the three source gases. The distributions can be fitted with exponentials of the form $\chi/\chi_{max} = \exp[-Az^n]$; for the neutrally buoyant plume, n = 1.5 and for the CO_2 plume, n = 1. In the outer portions of the SF_6 plumes, the value of n is approximately 0.6.

The vertical distributions of SF_6 and CO_2 for seven downwind distances have been scaled by the surface concentrations (χ_{max}) and by the distances to the points where the concentrations are 1% of the surface values ($z_{1/100}$) and replotted in Figures 5a (SF_6) and 5b (CO_2). The self-similarity in the profiles is strikingly apparent. Indeed, such self-similarity may seem unexpected; far downstream, where the density differences become insignificant, we might expect the plumes to diffuse as passive tracer material. For example, for SF_6 at x = 2500 mm, the source gas is diluted to 2% of its initial concentration at the surface. This implies a specific gravity of 1.08 (compared to the surrounding air), so that we might expect the density difference to have insignificant effect beyond that distance. However, the profiles remain self-similar well beyond that point, i.e., to at least 8500 mm downstream.

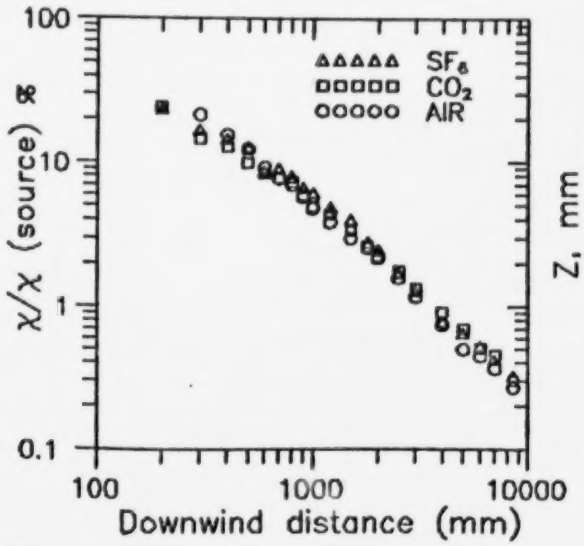

Fig. 3. Comparison of longitudinal concentration profiles of SF_6, CO_2, and air.

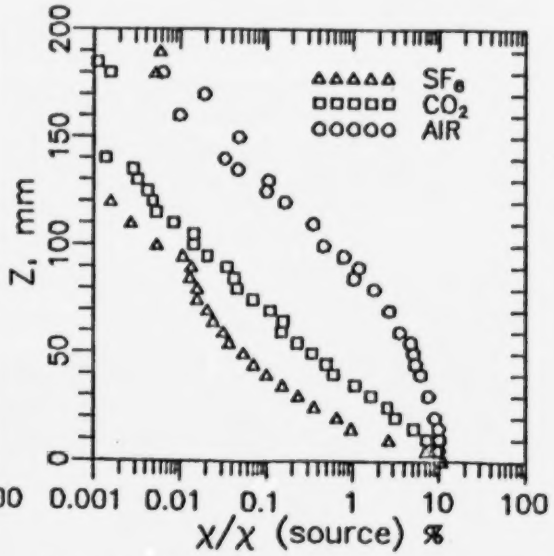

Fig. 4. Comparison of vertical concentration distributions of SF_6, CO_2 and air at x = 600 mm.

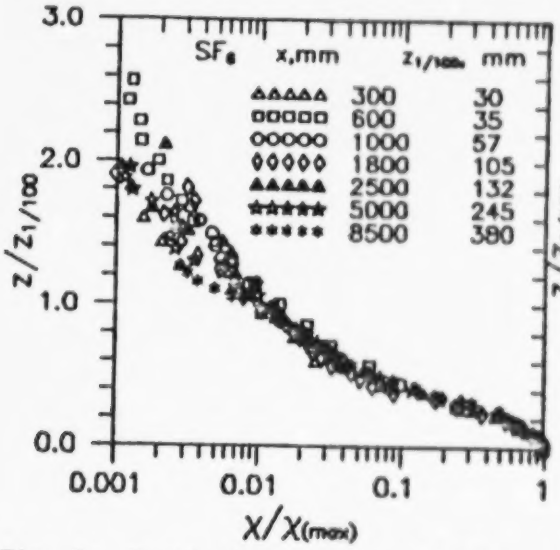

Fig. 5a. Vertical concentration profile of SF_6.

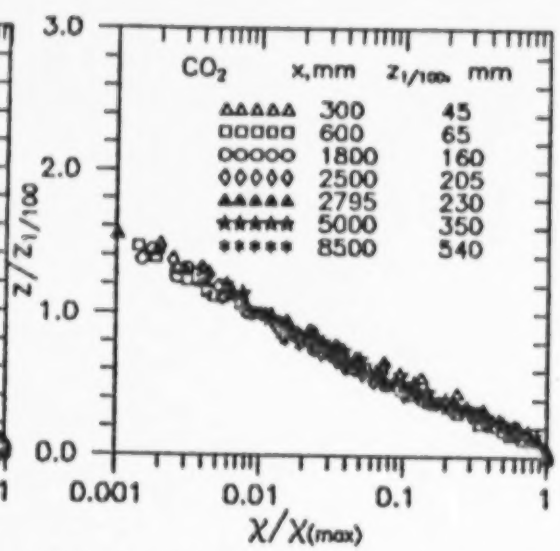

Fig. 5b. Vertical concentration profile of CO_2.

The lateral profiles of SF_6, CO_2, and air at 600 mm downwind are shown in Figures 6. The SF_6 plume is much wider than the CO_2 plume. Note that the two lateral profiles for SF_6 are displayed, one with an effective sampling height at 5 mm and the other at 0 mm. The profile measured at the 0 mm elevation shows considerably smaller scatter and up to a factor of 2 larger values of concentration. As discussed earlier, these differences were clearly due to the extremely steep concentration gradients close to the surface and near the source. Farther downstream, the vertical gradients approached zero, so that the differences in the profiles at the two elevations also approached zero. Note that the repeatability of the measurements is excellent. Two independently measured lateral profiles (at z = 5 mm), where the "scatter" in the sense of measurement reproducibility is generally within 2%. The apparent scatter is thus clearly related to

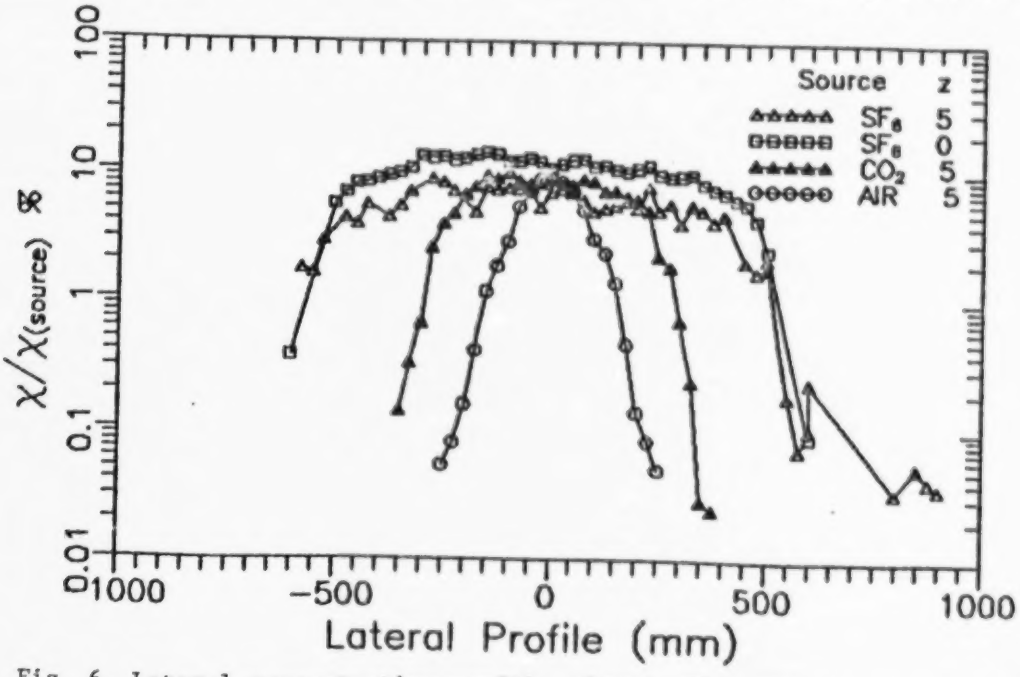

Fig. 6. Lateral concentration profile of SF_6, CO_2, and air at x = 600 mm.

the difficulty in precisely positioning a measurement probe above a rough surface.

BRIEF DESCRIPTION OF MODELS

Two models, INPUFF and DEGADIS, are chosen here to evaluate against the measured CO_2 and SF_6 concentrations. A brief description of each model is provided below.

INPUFF (Petersen and Lavdas, 1986) is a Gaussian Integrated Puff model which has a wide range of application. The model can be made to use a series of puffs to simulate a continuous plume. The dispersion coefficients used in the model can be chosen either from the P-G scheme or the on-site scheme for short travel times. For long travel times the dispersion of the puff is proportional to the square root of the travel time. In this study, the P-G scheme was used in determining the dispersion coefficients.

DEGADIS (Havens and Spicer, 1985) is a dense cloud model developed for the U.S. Coast Guard. The model treats the dispersion of the cloud in three distinct regimes, namely, buoyancy-dominated dispersion in the near field, stably stratified shear flow in the intermediate field, and passive turbulent dispersion in the far-field. The near-field buoyancy-dominated dispersion is modeled through gravity-spreading of the dense cloud and entrainment of the ambient air into the cloud by using an entrainment velocity. The downwind dispersion phase is modeled by assuming a power-law concentration distribution in the vertical direction and a modified Gaussian profile with a central homogeneous section in the horizontal direction together with a power-law for the vertical wind profile.

RESULTS AND DISCUSSION

Model runs were performed assuming a scale ratio of 1:100. For example, 500 mm in the wind tunnel scales to 50 m real scale. This scaling provided simulations for wind speeds that are of more interest than say a scale of 1:1000. The relevant dimensionless groups for modeling a steady release are U^2/gL, and q_o/UL^2, where U, g, q_o, and L are the wind speed at the top of the boundary layer, acceleration due to gravity, emission rate, and the height of boundary layer, respectively. To model at full scale, we require that these dimensionless ratios remain the same as those in the wind tunnel. The wind speeds were computed and extrapolated to a 10 m height assuming a wind profile exponent of 0.15, which is appropriate for neutral atmospheric conditions. The wind speeds used in the model runs for CO_2 and SF_6 were 6.7 m/s and 7.9 m/s respectively. The emission rates used in the model runs for CO_2 and SF_6 were 91.5 kg/s and 303.7 kg/s, respectively.

Figure 7 shows the observed and predicted centerline concentrations of SF_6 and CO_2 as functions of downwind distance from the source. INPUFF underestimated downwind concentrations for both SF_6 and CO_2 by about the same amount. DEGADIS simulated CO_2 dispersion well and performed about the same as INPUFF for SF_6.

Figure 8 shows the vertical profiles for the observed and predicted concentrations from DEGADIS and INPUFF at 60 m and 500 m downwind. The results for DEGADIS are in good agreement with the observations, while INPUFF underestimates the ground-level concentrations and as expected significantly overestimates concentrations aloft. In general, vertical profiles predicted by DEGADIS improved with downwind distance for both CO_2 and SF_6. These results suggest that the assumption of a Gaussian distribution for the vertical spread of the plume in a passive gas model such as INPUFF

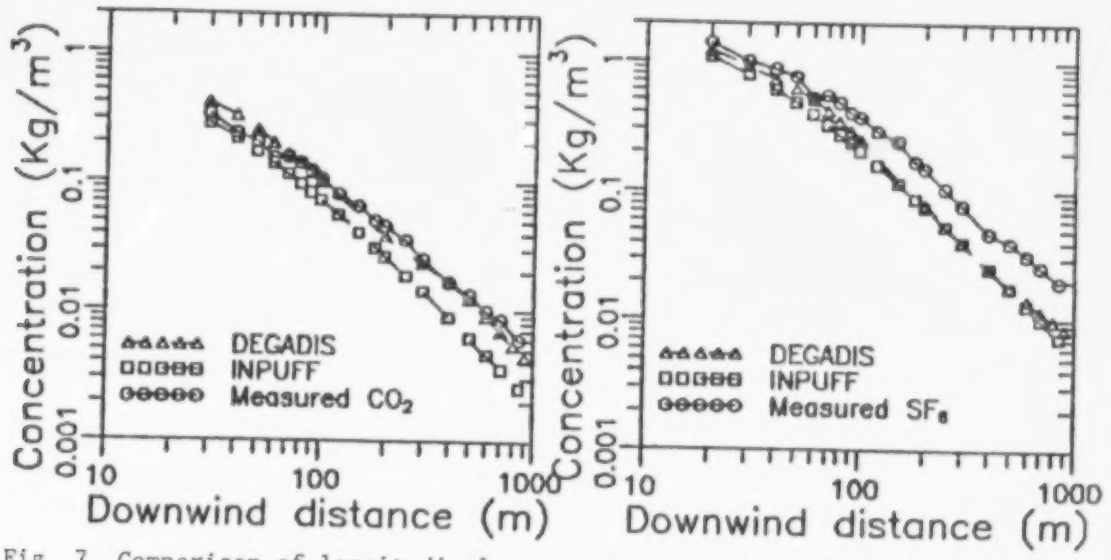

Fig. 7. Comparison of longitudinal concentrations of SF_6 and CO_2 with model estimates.

does not properly describe the vertical dispersion process for heavier-than-air gases.

Horizontal (crosswind) profiles for the observed and predicted concentrations from DEGADIS and INPUFF at 60 m and 500 m downwind are shown in Figure 9. Close to the source the measured CO_2 concentrations display a wider top-hat shape with sharp edges when compared with those predicted by DEGADIS and INPUFF. However, DEGADIS provides a good characterization of lateral spread in the near field for SF_6. The INPUFF plumes are narrower than those of the observed and the center-line concentrations are somewhat lower than their corresponding observed values. The reasonable agreement of the surface center-line concentrations is probably due to the model's enhanced vertical diffusion, a phenomenon discussed by Hanna (1983). At downwind distances beyond 250 m, crosswind profiles of model runs and observed CO_2 concentrations agree well, indicating that the profiles are near Gaussian in shape and dispersing as a passive release. The near Gaussian shape in the crosswind profiles is not observed for SF_6 until the plume has traveled 850 m.

CONCLUSIONS

The longitudinal decreases of surface concentrations for SF_6 and CO_2 are similar to those for passive releases. However, the plume shapes are significantly different. Heavy gas plumes are much wider and flatter. The vertical profiles of CO_2 are nearly exponential, whereas the exponent for the SF_6 profiles was clearly less than unity.

The results indicate that DEGADIS performs reasonably well in predicting the observed CO_2 concentrations and underestimates the SF_6 concentrations at greater downwind distances. This behavior suggest that DEGADIS needs improvement for the treatment of the plume lateral spread due to gravity effects. The Gaussian Puff model (INPUFF 2.2) overpredicts plume height and underpredicts the plume width. The combination of these effects results in an underestimation of the surface center-line concentrations. Also, the narrow plume estimated by the Gaussian puff model leads to an erroneous prediction of the off center-line concentrations values.

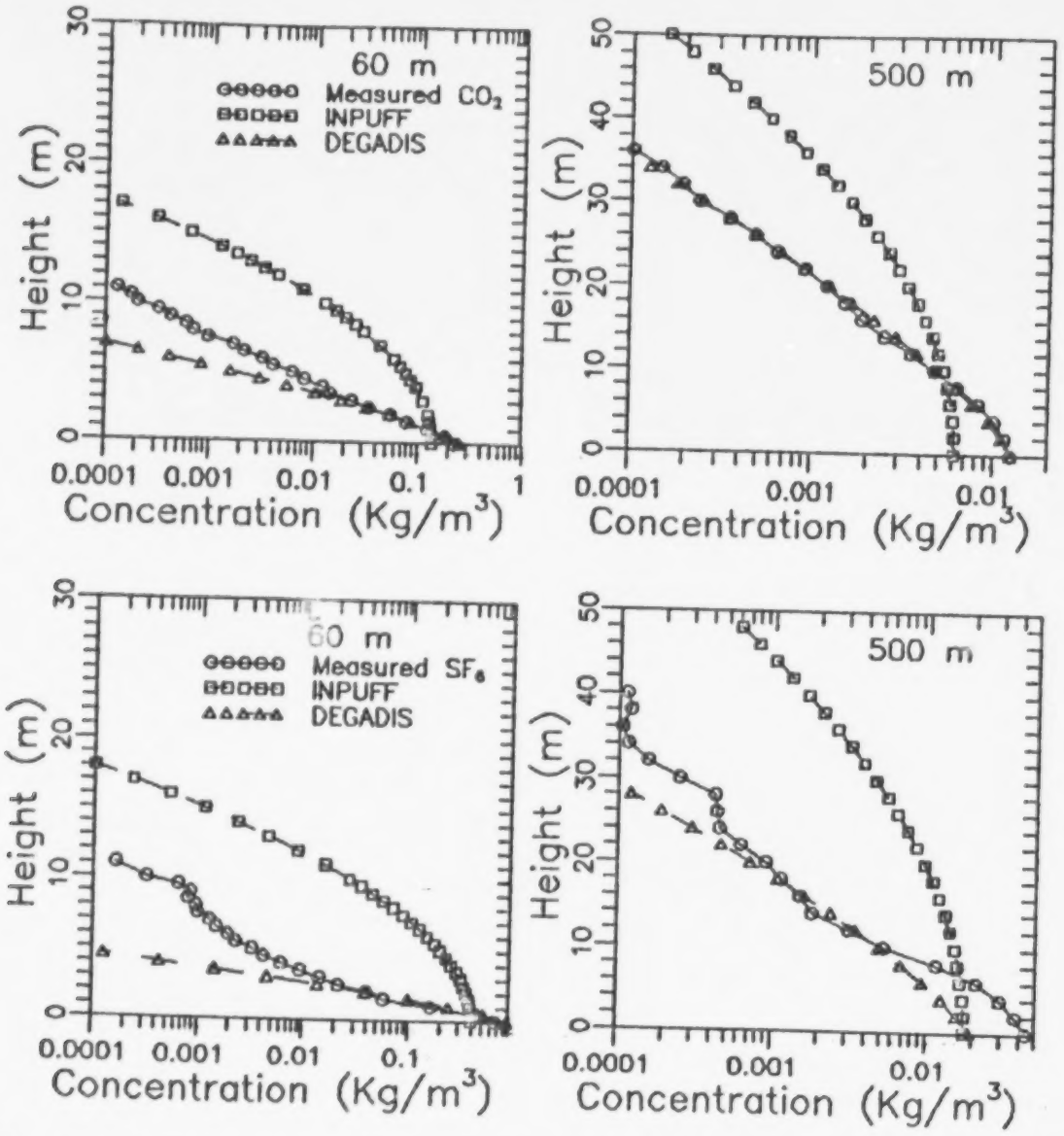

Fig. 8. Comparison of vertical concentration profiles of CO_2 (top 2 figures) and SF_6 (lower figures) with model estimates.

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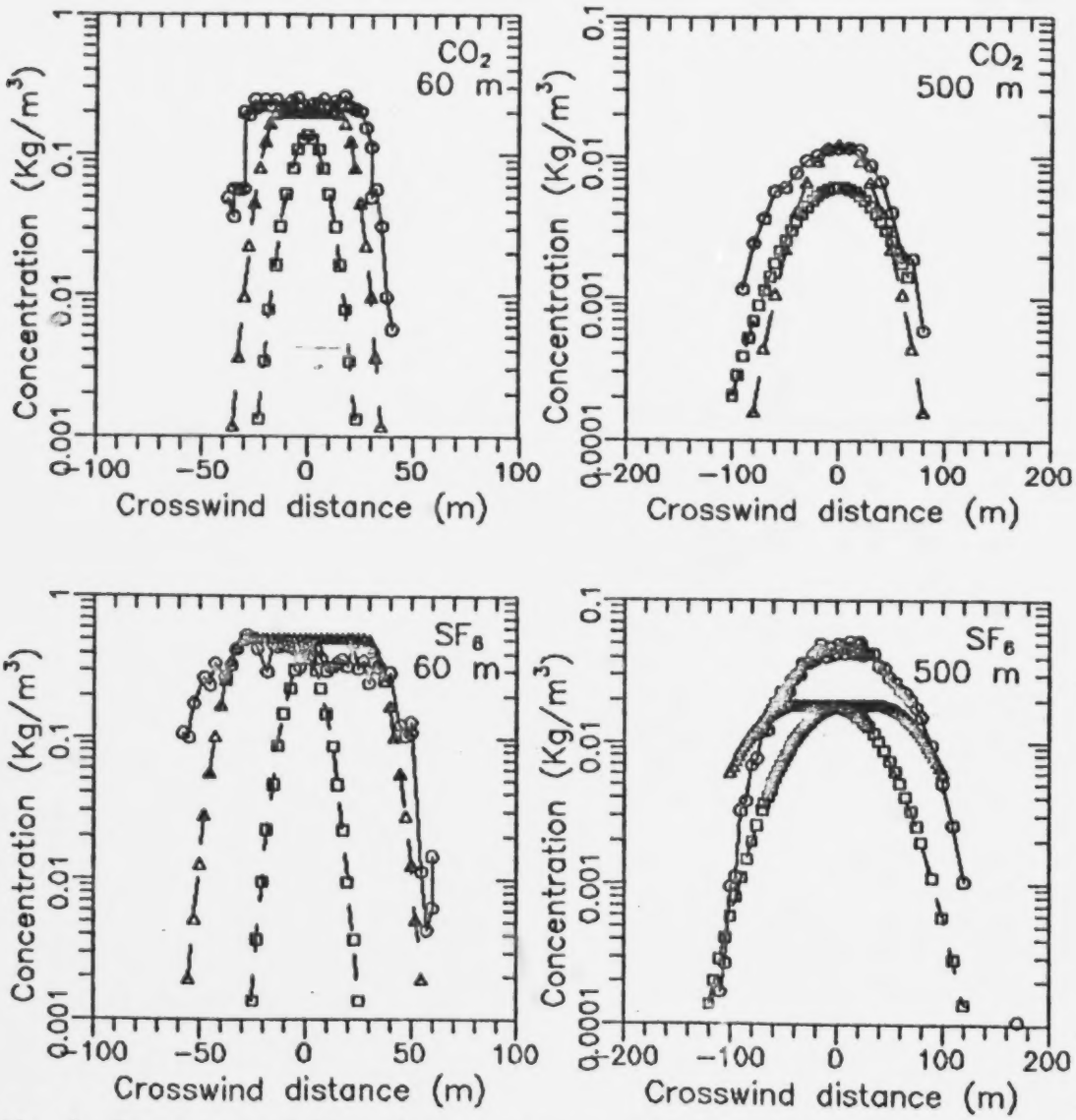

Fig. 9. Comparison of lateral concentration profiles of CO_2 (top figures) and SF_6 (lower figures) with model estimates. Circles, triangles, and squares are observations, DEGADIS estimates, and INPUFF estimates respectively.